Bayes Estimation of Common Parameters in Interlaboratory Studies

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Several materials measured by multiple laboratories – *two-way mixed model*

- Bayesian Model
- Likelihood Analysis
- Extension of Mandel-Paule Method
- Example

The Problem

- Each of p laboratories makes repeated measurements of m materials.

- The number of measurements made can differ among the laboratories, but each material is measured the same number of times by each laboratory.

- The within-laboratory variances can differ.

- The selected laboratories can be regarded as a random sample from an infinite population of laboratories.

How should one estimate 'consensus' values for the quantities measured, and what are the uncertainty in this estimates?

Example : Dietary Fiber
Li and Cardozo (1994)
J. Of AOAC Int., **77, p. 689**

Nine labs each measures fiber in *six* foods, in blind duplicates.

Sample	Laboratory			
	1	2	···	9
Apples	12.44	12.87	···	12.08
	12.48	13.20	···	12.38
Apricots	25.05	27.16	···	25.31
	25.58	26.29	···	25.43
⋮	⋮	⋮	···	⋮
FIBRIM	74.07	76.55	···	73.96
	75.01	78.36	···	74.24

Hierarchical Model With Noninformative Priors: Two-Way Model

$i = 1, \ldots, p$ indexes laboratories

$j = 1, \ldots, n_i$ indexes measurements

$k = 1, \ldots, m$ indexes materials

$$x_{ijk} = \theta_k + \epsilon_i + e_{ijk}$$

independent $\epsilon_i \sim \mathrm{N}(0, \sigma^2)$, $e_{ijk} \sim \mathrm{N}(0, \sigma_i^2)$.

$$p(x_{ijk} | \delta_i, \theta_k, \sigma_i^2) = \mathrm{N}(\delta_i + \theta_k, \sigma_i^2),$$

$$p(\sigma_i) \propto 1/\sigma_i,$$

$$p(\delta_i | \mu, \sigma^2) = \mathrm{N}(\mu, \sigma^2),$$

$$p(\theta_k) = 1,$$

can handle

$$p(\sigma_i) \propto \sigma_i^{\kappa_i}$$

Posterior of $(\{\theta_k\}, \sigma)$

Let T_ν and Z denote independent Student-t and standard normal random variables, and assume that $\psi \geq 0$ and $\nu > 0$. Then

$$U = T_\nu + Z\sqrt{\frac{\psi}{2}}$$

has *generalized t-distribution* with the density

$$f_\nu(u; \psi)$$

$$= \frac{1}{\Gamma(\nu/2)\sqrt{\pi}} \int_0^\infty \frac{y^{(\nu+1)/2-1} e^{-y\left[1+\frac{u^2}{\psi y+\nu}\right]}}{\sqrt{\psi y + \nu}} dy.$$

The posterior of $(\{\theta_k\}, \sigma)$ is

$$p(\{\theta_k\}, \sigma | \{x_{ijk}\}) \propto p(\sigma) \prod_{i=1}^{p} \frac{1}{t_i} f_{\nu_i}\left(\frac{\bar{x}_{i\cdot k} - \mu}{t_i}; \frac{2\sigma^2}{t_i^2}\right),$$

$\nu_i = n_i - 1$

$$t_i^2 = \frac{1}{\nu_i n_i m}[\sum_{j,k}(x_{ijk} - \bar{x}_{i\cdot k})^2$$

$$+n_i \sum_k (\bar{x}_{i\cdot k} - \bar{x}_{i\cdot\cdot})^2 + n_i \sum_k (\bar{\theta} - \theta_k)^2]$$

Given $\sigma = 0$, the posterior distribution of the consensus means θ_k is proportional to a product of scaled t-densities:

$$p(\theta_k | \{x_{ijk}\}, \sigma = 0) \propto \prod_{i=1}^{p} \frac{1}{t_i} T'_{n_i - 1}\left(\frac{\bar{x}_{i\cdot k} - \mu}{t_i}\right).$$

These densities reflect uncertainties in θ_k.

In the general case the posterior is proportional to the *product* of the appropriate generalized (symmetric) t-densities, centered at each lab average $\bar{x}_i$.

Matrix Formulation

A matrix formulation of the model: the ith laboratory repeats its vector measurements n_i times, the m-dimensional data $\{x_{ij}\}$ for $i = 1, \ldots, p$ and $j = 1, \ldots, n_i$ follow a two-way MANOVA model, which may be both unbalanced and heteroscedastic

$$x_{ij} = \theta + \epsilon_i + e_{ij}$$

independent $\epsilon_i \sim \mathrm{N}_m(0, \sigma^2 \mathbf{e}^{\mathbf{T}}\mathbf{e})$, $e_{ij} \sim \mathrm{N}_m(0, \Sigma_i)$, $j = 1, \ldots, n_i$.

Here $\mathbf{e}^{\mathbf{T}}\mathbf{e}$ is a covariance matrix (of rank one), and σ^2 is the unknown variance; θ represents unknown m-dimensional common to all laboratories mean; Σ_i^2 and σ^2 are the nuisance parameters.

A more general model,

$$x_{ij} = B_i[\theta + \epsilon_i] + e_{ij},$$

independent $\epsilon_i \sim \mathrm{N}_m(0, \sigma^2\Xi)$ $e_{ij} \sim \mathrm{N}_{m_i}(0, \Sigma_i)$.

The design matrices B_i have sizes $m_i \times m$, the known $m \times m$ matrix Ξ may have rank smaller than m, and θ represents unknown m-dimensional structural parameter common to all laboratories.

The covariance matrices Σ_i of size $m_i \times m_i$ and the unknown variance σ^2 are the nuisance parameters.

This model allows for the situation when some of the laboratories do not perform measurements on all components of θ, but rank $(B_i) \equiv m$.

For simplification in this talk $B_i \equiv \mathbf{I}$.

The statistics $x_i = \sum_{j=1}^{n_i} x_{ij}/n_i$, $S_i = \sum_{j=1}^{n_i}(x_{ij} - x_i)^T(x_{ij} - x_i)/\nu_i$ are sufficient.

The *generalized m-dimensional t-distribution* with density $f_\nu(u; \Psi)$ is that of the sum

$$U = V_\nu + Z$$

where independent $Z \sim \mathrm{N}_m(0, \Psi)$ and V has the density proportional to

$$\left[1 + v^T \times v\right]^{-(m+\nu)/2}$$

The posterior of (θ, σ) is

$$p(\theta, \sigma | \{x_{ij}\})$$

$$\propto p(\sigma) \prod_{i=1}^{p} \frac{1}{|T_i|} f_{\nu_i}\left(T_i^{-1}(x_i - \theta); 2\sigma^2 T_i^{-2}\Xi\right).$$

The same interpretation.

Likelihood Analysis

Put

$$\omega_i = \left[\frac{1}{n_i}\Sigma_i + \sigma^2\Xi\right]^{-1}.$$

The loglikelihood function can be written in the form

$$-2\ell = \sum_i (x_i - \theta)^T \omega_i (x_i - \theta) - \sum_i \log|\omega_i|$$

$$+ \sum_{i=1}^{p} \nu_i \log|\Sigma_i| + \sum_{i=1}^{p} \nu_i \mathrm{tr}\,(\Sigma_i^{-1} S_i) + C.$$

Local extreme points are possible. Cochran (1937), (1954), (1980). Vangel and Rukhin (1999)

The MLE of θ has the form

$$\widehat{\theta} = \left[\sum_{i=1}^{p} \omega_i\right]^{-1} \sum_{i=1}^{p} \omega_i x_i.$$

When Σ_i and σ are given, $\widehat{\theta}$ gives the optimal estimator of θ in the sense that it minimizes the sum of the mean squared errors

$$E(\tilde{x} - \theta)(\tilde{x} - \theta)^T$$

within the class of unbiased "linear estimators" $\tilde{x}$ of θ, $\tilde{x} = \sum_i A_i x_i$ with some matrices A_i. Thus it generalizes the classical weighted means statistics used when $m = 1$.

Extension of Mandel-Paule Method

Even without the normality assumption (only under existence of second moments) one has for $\widehat{\theta}$

$$E(x_i - \widehat{\theta})(x_i - \widehat{\theta})^T = \omega_i^{-1} - \left[\sum_{k=1}^{p} \omega_k\right]^{-1}.$$

$E(x_i - \widehat{\theta})^T \omega_i (x_i - \widehat{\theta})$ is a scalar,

$$\sum_{i=1}^{p} E(x_i - \widehat{\theta})^T \omega_i (x_i - \widehat{\theta})$$

$$= \sum_{i=1}^{p} \text{tr} \left(E(x_i - \widehat{\theta})(x_i - \widehat{\theta})^T \omega_i \right)$$

$$= \sum_{i=1}^{p} \text{tr} \left(\mathbf{I}_m - \left[\sum_{k=1}^{p} \omega_k \right]^{-1} \omega_i \right)$$

$$= mp - m = m(p-1).$$

This identity can be used as the estimating equation for θ and σ^2, provided that Σ_i are estimated by S_i.

This method consists in restricting the class of estimators of ω_i to those of the form $[n_i^{-1} S_i + y\Xi]^{-1}$ for some positive y. With the "weights"

$$w_i = w_i(y) = [n_i^{-1} S_i + y\Xi]^{-1},$$

an estimator of θ from this class has the representation

$$\widehat{x} = \widehat{x}(y) = \left[\sum_{i=1}^{p} w_i\right]^{-1} \sum_{i=1}^{p} w_i x_i.$$

The suggestion is to select the estimator out of this class, i.e. to choose y, which is designed to estimate σ^2, as the solution of the equation

$$\sum_{i=1}^{p} (x_i - \widehat{x})^T w_i(y)(x_i - \widehat{x}) = m(p-1). \quad (1)$$

A direct analogue of the Mandel-Paule algorithm widely used at NIST in the case $m = 1$. This is an easily implementable method suggested by Mandel and Paule (1970), Paule and Mandel (1982). It is known often to provide reasonable estimates. Schiller and Eberhardt (1992)- a discussion of this method as used in the preparation of standard reference materials.

This extension of the Mandel-Paule rule provides the estimate $\widehat{x}$ of the common parameter θ along with the estimate y of σ^2.

Properties:

- the Mandel-Paule rule is well defined, i.e. (1) has at most one positive solution;

- The left-hand side of (1) is a monotonically decreasing convex function.

Interpretation: an "approximate" version of the maximum likelihood estimator (or rather of the restricted maximum likelihood estimator)

$$\sum_{i=1}^{p} (x_i - \widehat{x})^T w_i(y)(x_i - \widehat{x}) = mp$$

This can be obtained from reparametrization of likelihood equation by estimating Σ_i by S_i,

which leads to the maximum likelihood estimate of σ^2 of the form

$$\widehat{\sigma}^2 \sim$$

$$y\frac{\sum_{i=1}^{p}(x_i-\widehat{\theta})^T\left(n_i^{-1}S_i+y\Xi\right)^{-1}(x_i-\widehat{\theta})+n-mp}{n}.$$

Thus the Mandel-Paule rule is characterized by the following fact:

$$\widehat{\sigma}^2 \sim y.$$

Rukhin and Vangel (1998)

To obtain a confidence set for θ assume that p is large. Under some conditions $\widehat{x}$ has approximately m-dimensional normal distribution with mean θ and the covariance matrix which can be estimated by

$$\Upsilon = \frac{1}{p}\left[\sum_{i=1}^{p} w_i\right]^{-1}$$

$$\left[\sum_{i=1}^{p} w_i(x_i-\widehat{x})(x_i-\widehat{x})^T w_i\right]\left[\sum_{i=1}^{p} w_i\right]^{-1}.$$

Provided Υ is nonsingular, one obtains an approximate $(1-\alpha)$-confidence ellipsoid for θ,

$$\left\{\theta : (\widehat{x}-\theta)^T \Upsilon^{-1} (\widehat{x}-\theta) \leq \chi^2_\alpha(m)\right\},$$

$\chi^2_\alpha(m)$ - α-critical point for the χ^2- distribution with m degrees of freedom.

The method extends to the situation when $\sum_i \omega_i$ may be non-invertible, as with $\left[\sum_{i=1}^p \omega_i\right]^-$ denoting the Moore-Penrose pseudoinverse,

$$\widehat{\theta} = \left[\sum_{i=1}^p \omega_i\right]^- \sum_{i=1}^p \omega_i x_i,$$

and

$$E(x_i - \widehat{\theta})(x_i - \widehat{\theta})^T = \omega_i^- - \left[\sum_{k=1}^p \omega_k\right]^-.$$

Then the equation (1) is to be re[placed by

$$\sum_{i=1}^p (x_i - \widehat{x})^T w_i(y)(x_i - \widehat{x}) = mp - q$$

with $q =$ rank $\left(\sum_{k=1}^p \omega_k\right)$.

Dietary Fiber in Apricots

Lab.	x_i	s_i^2	n_i
1	25.32	0.37	2
2	26.72	0.62	2
3	27.89	0.35	2
4	27.70	1.85	2
5	27.42	0.61	2
6	24.30	0.21	2
7	27.11	0.37	2
8	27.28	0.09	2
9	25.37	0.08	2

Mean: $\bar{x} = 26.567$

Weighted Means:

$$\begin{aligned} \text{MP} &= 26.472 \\ \text{ANOVA} &= 26.420 \\ \text{MLE} &= 27.275 \end{aligned}$$